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Tracing the Pareto frontier in bi-objective optimization problems by ODE techniques

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Abstract In this paper we present a deterministic method for tracing the Pareto frontier in non-linear bi-objective optimization problems with equality and inequality constraints. We reformulate the bi-objective optimization problem as a parametric single-objective optimization problem with an additional Normalized Normal Equality Constraint (NNEC) similar to the existing Normal Boundary Intersection (NBI) and the Normalized Normal Constraint method (NNC). By computing the so called Defining Initial Value Problem (Defining IVP) for segments of the Pareto front and solving a continuation problem with a standard integrator for ordinary differential equations (ODE) we can trace the Pareto front. We call the resulting approach *ODE NNEC method* and demonstrate numerically that it can yield the entire Pareto frontier to high accuracy. Moreover, due to event detection capabilities available for common ODE integrators, changes in the active constraints can be automatically detected. The features of the current algorithm are illustrated for two case studies whose `Matlab`® code is available as Electronic Supplementary Material to this article.

Keywords Bi-objective optimization · continuation method · deterministic multi-disciplinary optimization · Normal Boundary Intersection · Normalized Normal Constraint · numerical integration

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1 Introduction

Practical optimization problems often have multiple and conflicting objectives. In contrast to single-objective optimization (SOO) problems, these multiple objective optimization (MOO) problems give rise to a set of so-called *Pareto optimal* solutions instead of one single optimum [8]. To generate this Pareto set, the MOO problem is often reformulated as a series of parametric single-objective optimization (SOO) problems. The Pareto front is approximated by varying the reformulation parameters of the method involved. This class of methods includes the classic convex *Weighted Sum* (WS) of the different objectives, but also encompasses superior methods such as *Normal Boundary Intersection* (NBI) [4], or *Normalized Normal Constraint* (NNC) [7].

Tracking the solutions of these parametric SOO problems by continuation approaches (see, e.g., Allgower and Georg [1]) can be an attractive way to generate the Pareto frontier. Continuation strategies based on a WS reformulation have been proposed by, e.g., Rakowska et al. [9] for (inequality constrained) bi-objective optimization (BOO) problems, and by Hillermeier [6] for general (equality constrained) MOO problems. Numerically, continuation problems are often solved via general predictor-corrector algorithms. However, as continuation approaches for the BOO case also give rise to a system of ordinary differential equations (ODEs) with the reformulation parameter as independent variable, the use of standard integration routines instead of the specific predictor-corrector algorithms becomes particularly attractive. Moreover, since novel reformulations as NBI and NNC have been found to outperform the classic WS [4,7], incorporating these methods in continuation strategies which exploit standard integrators may be an appealing strategy for the solution of general BOO problems.

Therefore, the aim of the current paper is to provide a generic solution strategy for equality and inequality constrained BOO problems based on ODE techniques. Hereto, a Normalized Normal Equality Constraint (NNEC) reformulation similar to NBI and NNC is employed in order to obtain a parametric SOO problem. Then, the solutions of these parametric SOO problems are expressed as an ODE system, which is solved using standard integration routines (i.e., from the `Matlab`® ODE-suite [10]). We call the approach the *ODE NNEC method*. Furthermore, we provide the code for the examples treated in this paper as a template in Online Resource 1.

The paper is organized as follows. Section 2 states the BOO problem formulation and introduces several well-known parametric reformulations. Section 3 explains the proposed ODE based continuation method, which is illustrated in Section 4 for two case studies. Finally, Section 5 summarizes the main conclusions.

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2 Bi-objective optimization problems

2.1 Bi-objective optimization problem formulation

We shall consider the non-linear BOO problem with equality and inequality constraints

$$\min_{x\in\mathbb{R}^n} \{f_1(x), f_2(x)\}$$

subject to

$$\begin{aligned} g_i(x) &\leq 0, \quad i = 1, \ldots, m_{\text{ineq}}, \\ h(x) &= 0, \end{aligned}$$

with twice continuously differentiable functions $f : \mathbb{R}^n \to \mathbb{R}^2$, $g : \mathbb{R}^n \to \mathbb{R}^{m_{\text{ineq}}}$, and $h : \mathbb{R}^n \to \mathbb{R}^{m_{\text{eq}}}$. The first and second components f_1 and f_2 of f are competing objective functions. The inequality and equality constraints are given by the components of g and h, respectively. For notational convenience, the feasible design space $\mathcal{S}$ and the feasible objective space $\mathcal{F}$ are introduced as

$$\begin{aligned} \mathcal{S} &= \{x \in \mathbb{R}^n \,|\, g_i(x) \leq 0, i = 1, \ldots, m_{\text{ineq}}, \text{ and } h(x) = 0\}, \\ \mathcal{F} &= \{f(x) = [f_1(x), f_2(x)]^T \,|\, x \in \mathcal{S}\}. \end{aligned}$$

As for general MOO problems, the criterion to judge the optimality of possible solutions to this BOO is most often the concept of *Pareto optimality*.

Definition 1 A point $x^* \in \mathcal{S}$ is Pareto optimal iff there does not exist another point $x \in \mathcal{S}$ such that $f_i(x) \leq f_i(x^*)$ for $i = 1, 2$ and $f_i(x) < f_i(x^*)$ for at least one objective.

In other words, a feasible point is Pareto optimal (or *Pareto efficient*) if there exists no other feasible point that improves at least one objective function without worsening the other. Hence, it is clear that every Pareto optimal point has to lie on the boundary of the feasible objective space.

2.2 Parametric single-objective optimization problem reformulations

Over the past decades several techniques have been reported to convert the BOO problem into a series of parametric SOO problems.

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2.2.1 Weighted Sum

The most often employed technique in practice is combining the different objectives into a convex weighted sum, which results in the parametric SOO problem

$$\min_{x} f_{\mathrm{ws}}(x) = w_1 f_1(x) + w_2 f_2(x) \tag{1a}$$

subject to

$$g_i(x) \leq 0, \quad i = 1, \ldots, m_{\mathrm{ineq}}, \tag{1b}$$
$$h(x) = 0, \tag{1c}$$

with $w_1, w_2 \geq 0$ and $w_1 + w_2 = 1$. By consistently varying the weights w_1 and w_2 an approximation of the Pareto set is obtained. The WS approach is remarkably simple. However, it has several intrinsic drawbacks [3]. A uniform distribution of the weights does not necessarily result in an even spread on the Pareto front and points in non-convex parts of the Pareto set cannot be obtained.

2.2.2 Normal Boundary Intersection

This method has been proposed by Das and Dennis [4] to mitigate the above mentioned drawbacks of the WS approach. NBI tackles the BOO problem from a geometric viewpoint. It first builds a line in the objective space $\mathcal{F}$ which is determined by the minima for the problem with only a single objective f_i, i.e., the *convex hull of individual minima* (CHIM), and then constructs *(quasi-)normal* lines to the CHIM. The rationale behind the method is that the intersection between the (quasi-)normal from any point f_p on the CHIM, and the boundary of the feasible objective space closest to the origin is expected to be Pareto optimal. Hereto, the BOO objective problem is reformulated as to maximize the distance λ from a point f_p on the CHIM along the quasi-normal through this point, without violating the original constraints. Technically, this requirement of lying on the quasi-normal introduces additional equality constraints, resulting in the formulation

$$\max_{x,\lambda} \lambda \tag{2a}$$

subject to

$$g_i(x) \leq 0, \quad i = 1, \ldots, m_{\mathrm{ineq}}, \tag{2b}$$
$$h(x) = 0, \tag{2c}$$
$$\Phi w - \lambda \Phi e = f(x) - f^*, \tag{2d}$$

where Φ is the 2×2 pay-off matrix in which the i-th column is $f(x_i^*) - f^*$, with x_i^* being the minimizer of the i-th objective f_i and f^* being the utopia point, which contains the minima of the individual objectives $f_i(x_i^*)$. The vector of weights $w = [w_1, w_2]^T$ is such that $w_1 + w_2 = 1$ with $w_1, w_2 \geq 0$, and e is a vector containing all ones. Now, Φw describes a point f_p on the CHIM and $-\Phi e$ defines the (quasi-)normal to the CHIM pointing towards the origin. When the points on the CHIM are chosen on an equidistant grid of $[0, 1]$ for w_1, the sample points on the Pareto frontier in the objective space are in general better distributed than in the WS approach.

2.2.3 Normalized Normal Constraint

NNC as introduced by Messac et al. [7] employs ideas similar to NBI, but combines them with features of the ε-constraint method [5]. This ε-constraint method minimizes the single most important objective function f_k, while the other objective function is added as an inequality constraint $f_i \leq \varepsilon_i$, which is interpreted as a halfplane reducing the feasible objective space. After normalization of the objectives, NNC also first constructs a line through the individual minima (called the *utopia line* here). Then, NNC minimizes a selected (normalized) objective $\bar{f}_k$, given the original constraints, and while additionally reducing the feasible objective space by adding a halfplane through a selected point $\bar{f}_p$ on the utopia line. This halfplane is chosen perpendicular to the *utopia line*. Thus, this approach leads to an additional inequality constraint, resulting in the optimization problem

$$\min_x \bar{f}_k \tag{3a}$$

subject to

$$
\begin{aligned}
g_i(x) &\leq 0, \quad i = 1, \ldots, m_{\text{ineq}}, &\text{(3b)}\\
h(x) &= 0, &\text{(3c)}\\
(\bar{f}(x_k^*) - \bar{f}(x_i^*))^T (\bar{f}(x) - \bar{f}_p) &\leq 0, \quad i = 1, 2, i \neq k. &\text{(3d)}
\end{aligned}
$$

As in NBI, evenly distributed points on the utopia line $\bar{f}_p$ can be selected by a uniform variation of a vector w, which also ensures an even spread on the Pareto set.

3 Continuation based tracking of the Pareto frontier

Often, a-priori discretizations of the NBI and NNC parameters w are chosen. Although better than WS approaches, this may still result in rather coarse approximations of the Pareto set, as will be shown in Section 4. In the current study, a continuation method is used to track the Pareto front with high accuracy. The continuation problem is treated by solving the Defining Initial Value Problem (Defining IVP, see, e.g., [1]) with standard integration tools. The rationale behind the proposed method is to first employ *a reformulation*

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approach similar to NBI and NNC in order to obtain a parametric SOO problem in one reformulation parameter α (see Section 3.1). The solutions of this parametric SOO problem for all parameters $\alpha \in [0, 1]$ are obtained by *integrating an ODE system with the parameter α as independent variable.* This ODE system is derived from the *first-order necessary conditions of optimality for the parametric SOO problem* and the *Implicit Function Theorem* (see Section 3.2). Due to the presence of inequality constraints, changes in the active constraints have to be detected and the *active set has to be updated* accordingly (see Section 3.3). In practice, event detection features of standard numerical integration schemes can be exploited for this purpose. However, as the current approach tracks the boundaries of the feasible objective space only locally, non-Pareto optimal parts may have to be removed in a post-processing step by a *Pareto filter algorithm* (see Section 3.4).

Without loss of generality, it will be assumed in the remainder of this paper that both objective functions have been normalized and we shall omit the bars $\bar{\cdot}$ for notational convenience.

We shall now outline the ODE NNEC method:

1. Compute the two individual minima.
2. For the initial value of the reformulation parameter, e.g., $\alpha = 0$, find the corresponding active set and the Lagrange multipliers.
3. Integrate the Defining Initial Value Problem until a change in the active set occurs or until $\alpha = 1$.
4. If a change in the active set is detected, then find the new active set, compute the corresponding Lagrange multipliers, and return to Step 3.
5. If $\alpha = 1$, then terminate.
6. If necessary, apply a Pareto filter algorithm (see, e.g., [7]).

In the following sections, the different steps are elaborated.

3.1 Parametric single-objective optimization reformulation

As NNC, the NNEC reformulation aims at minimizing one of the normalized objectives, i.e., f_2. It also constructs the *utopia vector* $u = f(x_2^*) - f(x_1^*) = [1, -1]^T$ and its *normal* $n = [1, 1]^T$, based on the individual minima $f(x_1^*) = [0, 1]^T$ and $f(x_2^*) = [1, 0]^T$. Hence, any point on the *utopia line* (joining the two individual minima) can be written as

$$f_p(\alpha) = \alpha f(x_1^*) + (1 - \alpha) f(x_2^*) = [1 - \alpha, \alpha]^T$$

and any point orthogonal to this line is given by the relation

$$u^T (f(x) - f_p(\alpha)) = u^T f(x) - 1 + 2\alpha = 0.$$

In NNC, the last expression contains an inequality instead of an equality sign in order to reduce the feasible region by adding a halfplane. However, in the current approach, the equality is kept. Hence, the solution point has to be

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part of the normal to the utopia line (or CHIM), similar to the NBI approach. In summary, the original BOO problem is converted to the parametric SOO problem (SOO$_\alpha$)

$$\min_x f_2(x)$$

subject to

$$\begin{aligned} g_i(x) &\leq 0, \quad i = 1, \ldots, m_{\text{ineq}}, \\ h(x) &= 0, \\ u^T(f(x) - f_p(\alpha)) &= 0. \end{aligned}$$

3.2 ODE system for the continuation strategy

In general, the set of α-dependent solutions of (SOO$_\alpha$) can consist of several segments according to the different sets of active inequality constraints. Hence, on a segment with a constant active set $\mathcal{A}(x) = \{i \,|\, g_i(x) = 0\}$, this leads to the following parametric subproblem (ASP$_\alpha$) :

$$\min_x f_2(x)$$

subject to

$$\begin{aligned} g_i(x) &= 0, \quad i \in \mathcal{A}(x), \\ h(x) &= 0, \\ u^T(f(x) - f_p(\alpha)) &= 0. \end{aligned}$$

Defining the Lagrangian

$$L(x, \lambda, \mu, \mu_e) = f_2(x) + \lambda_{\mathcal{A}(x)}^T g_{\mathcal{A}(x)}(x) + \mu^T h(x) + \mu_e u^T(f(x) - f_p(\alpha))$$

allows to specify the first-order necessary conditions for optimality

$$F(x, \lambda_{\mathcal{A}}, \mu, \mu_e, \alpha) = \begin{bmatrix} \nabla_x L \\ g_{\mathcal{A}} \\ h \\ u^T(f - f_p(\alpha)) \end{bmatrix} = 0.$$

When denoting $[x, \lambda_{\mathcal{A}}, \mu, \mu_e]^T$ as y, the Jacobian of F with respect to y is given by the expression

$$\frac{\partial F}{\partial y} = \begin{bmatrix} \nabla_{xx} L & \nabla g_{\mathcal{A}} & \nabla h & \nabla f u \\ \nabla g_{\mathcal{A}}^T & 0 & 0 & 0 \\ \nabla h^T & 0 & 0 & 0 \\ u^T \nabla f^T & 0 & 0 & 0 \end{bmatrix}.$$

Under the assumption that this Jacobian matrix is invertible at (y_0, α_0), the *Implicit Function Theorem* yields the existence of a neighborhood $U_y \times U_\alpha$ of

(y_0, α_0) and a function $y : U_\alpha \to U_y$ such that $F(y(\alpha), \alpha) = 0$ for all $\alpha \in U_\alpha$. It also provides that $y(\alpha)$ is continuously differentiable in U_α with

$$\frac{\mathrm{d}y}{\mathrm{d}\alpha} = -\left(\frac{\partial F}{\partial y}\right)^{-1}\frac{\partial F}{\partial \alpha} = -\begin{bmatrix} \nabla_{xx}L & \nabla g_{\mathcal{A}} & \nabla h & \nabla f u \\ \nabla g_{\mathcal{A}}^T & 0 & 0 & 0 \\ \nabla h^T & 0 & 0 & 0 \\ u^T \nabla f^T & 0 & 0 & 0 \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 2 \end{bmatrix} =: -K(y)^{-1} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 2 \end{bmatrix}. \tag{4}$$

Equation (4) defines an ODE system with the parameter α as independent variable and $y = [f, x, \lambda_{\mathcal{A}}, \mu, \mu_e]^T$ as dependent variables. For suitable initial conditions, this ODE system can be integrated resulting in one segment of the Pareto frontier.

The question of invertibility of $\partial F/\partial y$ remains to be discussed. Necessarily, $\nabla f u \neq 0$ must hold. Geometrically, this is equivalent with the condition that the Pareto front is not parallel with the utopia normal u. Furthermore, we want to assume that the submatrix

$$\begin{bmatrix} \nabla_{xx}L & \nabla g_{\mathcal{A}} & \nabla h \\ \nabla g_{\mathcal{A}}^T & 0 & 0 \\ \nabla h^T & 0 & 0 \end{bmatrix}$$

is invertible, because otherwise problem (SOO$_\alpha$) would not have a unique solution for some $\alpha \in [0, 1]$. Therefore, $\partial F/\partial y$ is invertible if $\nabla f u$ is linear independent of the columns of $\begin{bmatrix} \nabla g_{\mathcal{A}} & \nabla h \end{bmatrix}$, or, geometrically speaking, the tangent of the Pareto front is not parallel to the tangent space of the equality and active inequality constraints.

In a numerical code, however, mere invertibility is not sufficient for the reliable solution of an IVP for ODE (4). The adaptive components of an IVP solver will lead to tiny step-sizes if the matrix $K(y)$ is badly conditioned, which is often the case for optimization problems in real-world applications. Solving instead the equivalent implicit ODE

$$K(y)\frac{\mathrm{d}y}{\mathrm{d}\alpha} = [0, 0, 0, -2]^T \tag{5}$$

with an implicit numerical integration method avoids small step-sizes and leads to higher efficiency for badly conditioned problems.

3.3 Active set determination

The ODE system (4) must be reformulated when the active set changes (see [9]). Such changes can be detected as events, i.e., sign changes, in the *switching function*

$$\sigma(y) = [g_{\bar{\mathcal{A}}}(x), \lambda_{\mathcal{A}}]^T,$$

with $\bar{\mathcal{A}} = \{i \,|\, g_i(x) \neq 0\}$, the complement of $\mathcal{A}$. Here, a sign change from negative to positive values in one of the functions of $g_{\bar{\mathcal{A}}}(x)$, reveals that an additional inequality becomes active, and, hence, has to be added to the active set. Additionally, if one of the Lagrange multipliers of the active set $\lambda_{\mathcal{A}}$ becomes negative, one of the active inequalities becomes inactive, and, thus, has to be removed from the active set.

Whenever a switch in the switching function $\sigma(y)$ occurs, the active set has to be modified and new values for the Lagrange multipliers have to be computed. Thus, when the end of a segment is reached at a point x_e, $\mathcal{Z} = \{i \,|\, g_i(x_e) = 0\}$ defines the set of all possibly active inequalities. At the same point let

$$A = \begin{bmatrix} \nabla g_{\mathcal{Z}}^T \\ \nabla h^T \\ u^T \nabla f^T \end{bmatrix}$$

and let $r = \operatorname{rank}(A)$ denote the rank of A. Now, a new active set $\mathcal{A} \subset \mathcal{Z}$ has to be selected based on the following conditions:

1. The rank remains unaltered, i.e.,
$$\operatorname{rank}(\tilde{A}) = r \quad \text{ with } \tilde{A} = \begin{bmatrix} \nabla g_{\mathcal{A}}^T \\ \nabla h^T \\ u^T \nabla f^T \end{bmatrix}.$$
2. There exists $\lambda_{\mathcal{A}} \geq 0$ such that the first-order optimality conditions
$$\tilde{A}^T [\lambda_{\mathcal{A}}, \mu, \mu_e]^T = -\nabla f_2$$
are (still) satisfied.
3. None of the inequality constraints will be violated when tracing the segment in the direction of increasing α, i.e.,
$$\frac{\mathrm{d}g_i}{\mathrm{d}\alpha} = \nabla g_i^T \frac{\mathrm{d}x}{\mathrm{d}\alpha} \geq 0, \quad i \in \mathcal{Z}.$$

Whenever such an active set and the corresponding Lagrange multipliers have been found, the integration can be restarted to compute the next segment of the Pareto frontier.

3.4 Pareto filter

As non-Pareto optimal points can be returned by the ODE routine, these segments have to be removed from the final solution. However, due to the use of the ODE integrator, the resulting path of objective vectors f can be evaluated for any α. Thus, for a given set of α values, the corresponding set of objective vectors f can be processed by a Pareto filter algorithm, which removes the non-Pareto optimal points. This filtering is most often based on a pointwise comparison of the different Pareto candidates (see, e.g., [7]). Moreover, it is possible to refine the solution iteratively by each time refining the set of α values in the neighbourhood of interesting parts of the Pareto set (e.g., the end of a convex segment) and applying the Pareto filter.

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3.5 Implementation

We implemented the ODE NNEC method in the widely-used package `Matlab`® (The MathWorks Inc., Natick). The `Matlab`® ODE suite [10] has been employed for numerical integration of the Defining IVP with event detection for the active set. More specifically, we selected the explicit Dormand-Prince Runge-Kutta integrator `ode45` to solve IVPs for the explicit ODE (4) and the NDF-formula `ode15s` for IVPs of the implicit ODE (5). We want to remark that for these higher order methods the functions f, g, and h must be smooth enough, e.g., seven times continuously differentiable, otherwise the estimators for the local truncation error might fail and lead to tiny step-sizes. The problems treated in this article are all smooth enough. For problems which are not smooth enough one should use `ode15s` with a maximum order one smaller than the differentiability index, e.g., with a maximum order of one for problems with only twice continuously differentiable functions.

4 Results

In this section we illustrate the ODE NNEC algorithm. The results were obtained with an absolute and relative tolerance of 0.0001 and conservative initial stepsize suggestions of 0.01.

4.1 Case study

We shall discuss two examplary cases in this section.

4.1.1 Case I

The first case is based on the example from [7] to which an additional circle inequality constraint (6b) has been added in order to illustrate the active set tracking features. The resulting bi-objective optimization problem is

$$\min_{x\in\mathbb{R}^2}\{x_1, x_2\} \tag{6a}$$

subject to

$$\begin{aligned} 14 - x_1^2 - x_2^2 &\leq 0, &(6b)\\ 5e^{-x_1} + 2e^{-0.5(x_1-3)^2} - x_2 &\leq 0, &(6c)\\ x_1 - 5 &\leq 0, &(6d)\\ x_2 - 5.1 &\leq 0. &(6e)\end{aligned}$$

Figure 1 depicts the Pareto front generated with the explicit version of the proposed ODE NNEC method. It consists of three segments divided by kinks, corresponding to different active sets. We normalized the feasible objective

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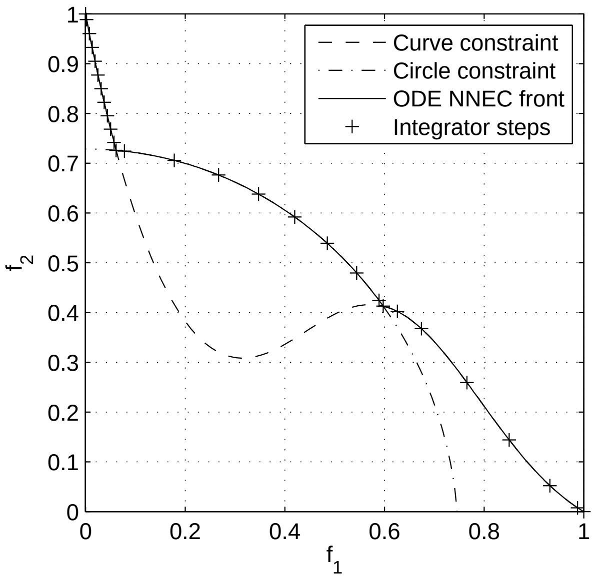

Fig. 1 Pareto front of Case I. The + signs denote the `ode45` integrator steps. The coordinates have been transformed such that the feasible objective space is normalized.

space. The + signs mark the steps of the ODE integrator. Because of the simplicity of the objective functions, the constraints can be directly mapped to the feasible objective space. We see that the non-convex Pareto front is accurately resolved. Especially, the points of changing active sets are precisely determined. This is an important advantage because these kinks are features which may be of distinguished importance to the decision maker. Furthermore, the Pareto front is non-convex in the middle which would have been impossible to resolve without manual restarts in a WS approach.

4.1.2 Case II

The second case has been taken from [3] in order to illustrate the presence of equality constraints. The problem is

$$\min_{x\in\mathbb{R}^5}\{x_1^2+x_2^2+x_3^2+x_4^2+x_5^2, 3x_1+2x_2-\frac{x_3}{3}+0.01(x_4-x_5)^3\} \tag{7a}$$

subject to

$$x_1+2x_2-x_3-0.5x_4+x_5-2=0, \tag{7b}$$
$$4x_1-2x_2+0.8x_3+0.6x_4+0.5x_5^2=0, \tag{7c}$$
$$x_1^2+x_2^2+x_3^2+x_4^2+x_5^2-10\leq 0. \tag{7d}$$

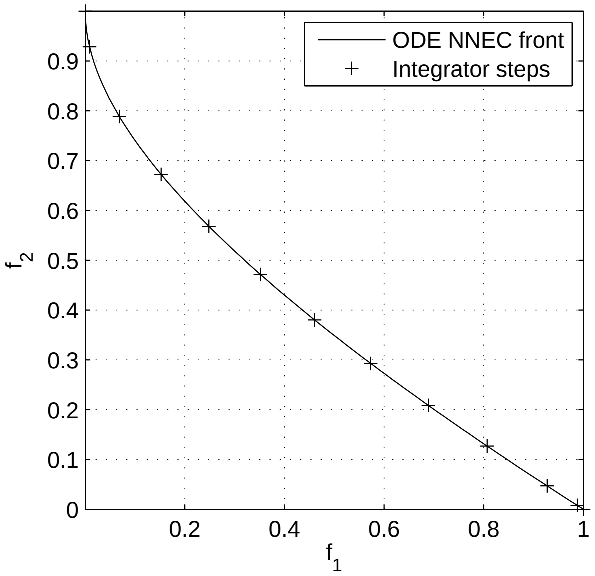

Fig. 2 Pareto front of Case II. The + signs denote the `ode45` integrator steps. The coordinates have been transformed such that the feasible objective space is normalized.

Figure 2 depicts the Pareto front generated with the ODE NNEC method. Consisting of only one segment, it is much simpler than the Pareto front of Case I. In fact the inequality constraint (7d) is only active in the lower right point of the Pareto front. Because the objective functions are more complicated than in Case I, there is no intuitive way of representing the constraints in the feasible objective space.

4.2 Comparison of the ODE NNEC method with the NBI method

We computed the accuracy of the solutions obtained with the proposed ODE NNEC approach in the two examples by comparison with reference solutions. For the first case, we used the analytical expressions for the constraints (6b) and (6c) limiting the feasible criterion space (and also providing the Pareto front). For the second case we computed the Pareto front with the explicit ODE NNEC method and tight integration tolerances (i.e., 10^{-13}). The difference of the normalized objective functions values of the reference solution and the final point $[0, 1]^T$ was $1.1 \cdot 10^{-14}$.

We carried out an additional comparison with solutions obtained by the NBI method [4]. For the numerical solution of problem (2) we used the active-set version of `fmincon`, an implementation of a Sequential Quadratic Programming (SQP) method contained in the Matlab Optimization Toolbox™ [2]. A hot-start strategy exploiting the solution of the previous NBI subproblem to

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	Case I	Case II	Case I	Case II
	Explicit ODE NNEC		Implicit ODE NNEC	
Integrator steps	30	13	57	26
Right hand side evaluations	177	73	194	96
Linear system solves	177	73	146	156
Linear system decompositions	177	73	30	18
$\|e(\alpha)\|_2$	6.8E-6	1.7E-7	2.7E-4	8.3E-5
$\|e(\alpha)\|_\infty$	4.8E-5	2.1E-6	6.3E-4	9.8E-5
	NBI		NBI	
Evaluation points (a priori)	82	31	57	75
SQP iterations	177	75	146	156
$\|e(\alpha)\|_2$	1.1E-4	2.9E-4	2.4E-4	6.4E-5
$\|e(\alpha)\|_\infty$	5.9E-3	1.8E-3	8.3E-3	2.9E-4

Table 1 Quantitative results for the ODE NNEC and NBI methods for the Cases I and II.

initialize the next one was implemented in order to speed up convergence. The optimality tolerance was set to 0.0001.

To facilitate a fair comparison, we selected the number of NBI points such that the total number of SQP iterations to compute the whole front was approximately the same as the total number of right hand side evaluations required for the explicit ODE NNEC method. For the implicit ODE NNEC method, we chose the number of NBI points to be approximately the number of linear system solves. The rationale behind this assumption is that every SQP iteration requires at least one formulation, decomposition, and solution of a linear system $K(y)$, which is, just as in the ODE NNEC method, the computational bottleneck. More than one linear system formulation, decomposition, and solution in one SQP iteration occurs only if the active set changes. The hot-start strategy for the NBI subproblems ensures that the SQP method is in most cases started with the correct active set. Thus, our choice for the number of NBI points is fair with respect to numerical effort, although slightly in favor of NBI.

Table 1 summarizes the results for the explicit and implicit versions of the ODE NNEC method and the NBI method. As explained above, the number of linear system solves required is on purpose approximately the same as the number of SQP iterations. These values correspond to a number of *evaluation points*, i.e., the number of integrator steps and the number of NBI subproblems, respectively. However, NBI does not provide information for the computation of the Pareto front in between the evaluation points. We use linear interpolation to obtain intermediate points. The NBI points cannot be used for higher order interpolation because this would introduce high errors around Pareto front kinks which are not identified automatically by the NBI method. On the other hand, the ODE NNEC method can exploit the high order interpolation polynomials employed in the integration scheme in order to compute intermediate points with high accuracy, but with negligible additional computational effort. This feature is also reflected in the L_2 and L_∞ error estimates $\|e(\alpha)\|_2$ and $\|e(\alpha)\|_\infty$. Here, the approximation error $e(\alpha)$ between the method's and the reference solution is measured at 1000 equally distributed sampling points along the Pareto front and is each time based on the distance in the $[1, 1]^T$ direction. This direction has been selected in order not to favor either of the two (normalized) objectives.

As was concluded from the Figures 1 and 2, both approaches yield an acceptable approximation of the Pareto front. However, the explicit ODE NNEC method outperforms the NBI method with respect to the global error $\|e(\alpha)\|_2$ as well as the maximum deviation $\|e(\alpha)\|_\infty$ with one to three orders of magnitude in accuracy. The reasons are twofold. First, the active set change detection procedure allows to locate kinks in the Pareto front very accurately in contrast to the smoothed piecewise linear approximations between NBI solution points. This feature is illustrated in the left plot of Figure 3, in which one of the two kinks in the Pareto set of Case I is displayed. Second, the high order polynomials allow a more accurate approximation in highly curved regions of the Pareto front than linear interpolation between the NBI solution points. The right plot of Figure 3 illustrates this property for the objective space region close to $[0, 1]^T$ in Case II.

The implicit ODE NNEC method yields an accuracy which is comparable to the NBI method for both error measures in Case II. In the more difficult Case I, the implicit ODE NNEC method is an order of magnitude better than NBI in the L_∞ norm, while the error in the L_2 norm is comparable. The regarded optimization problems are well-conditioned and we can conclude that it is advantageous to use the explicit version of ODE NNEC in that case.

However, we want to remark that the number of required linear system formulations and decompositions needed in the implicit ODE NNEC method is much smaller than the number of linear system solves. Thus, the implicit ODE NNEC method may be favorable also with respect to numerical efficiency on other examples.

4.3 Discussion

In this section we want to summarize the advantages and limitations of the proposed ODE NNEC method. One advantage is the applicability to a wide range of bi-objective optimization problems with equality and inequality constraints. Another advantage is the high accuracy with which convex and non-convex Pareto fronts can be efficiently computed. In case of connected Pareto sets and a bijective relation between the reformulation parameter and the points on the Pareto frontier, the entire Pareto set is automatically obtained without manual restarts. The automatic and accurate determination of active set changes may be very interesting for the decision maker, as they reveal intrinsic changes in the palette of Pareto optimal solutions. Finally, no advanced software is required, since only off-the-shelf components (e.g., the `Matlab`® ODE suite) are used.

We want to conclude this section with the limitations of the proposed method. The main drawback is the restriction to only two objectives. Continuation strategies for multi-objective optimization with more than two objec-

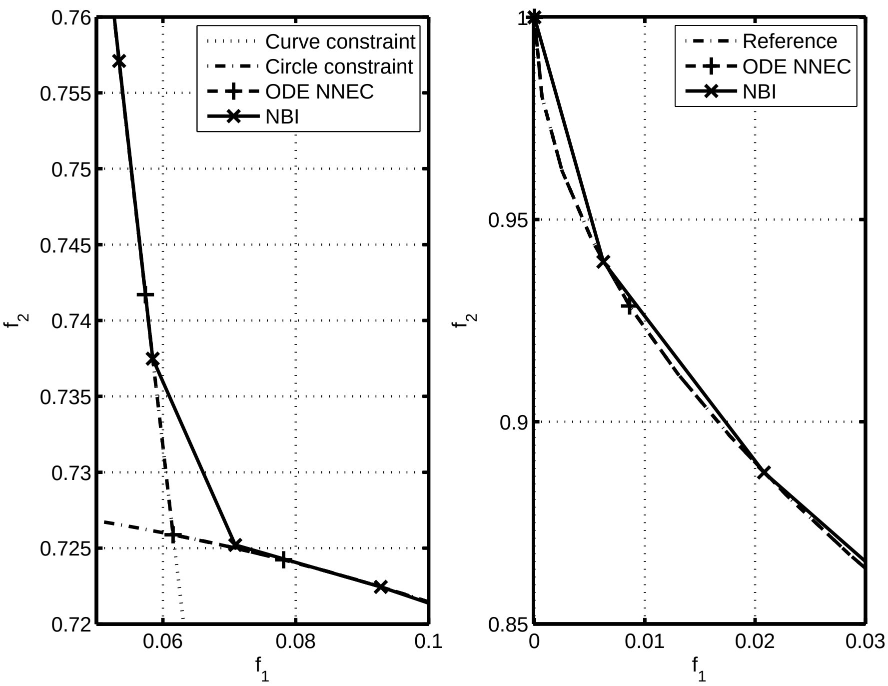

Fig. 3 Parts of the normalized objective space with Pareto sets for the reference solution, the ODE NNEC and NBI methods: Region around the first Pareto set kink in Case I (left), and region close to $[0, 1]^T$ in Case II (right).

tives cannot be realized with ODE techniques and one has to recede to more complicated procedures (see [6]). The ODE NNEC method shares a disadvantage with other local derivative based methods, namely, that problems occur when the reformulated parametric SOO exhibits several local minima for a single value of the reformulation parameter. Moreover, also due to the local character, non-Pareto optimal points can also be returned. However, since the Pareto curve can be obtained at any desired accuracy, regions with dominated points can accurately be removed with a Pareto filter algorithm [7].

5 Conclusion

We have presented the ODE NNEC method for tracing the Pareto frontier in non-linear bi-objective optimization problems with equality and inequality constraints. The method is based on deterministic, derivative based optimization principles, and on reformulation of the bi-objective optimization problem as a parametric single-objective problem with a normalized normal equality constraint. We solve the parametric problem for the whole range of parameters with a continuation approach, by formulating the Defining Initial Value Problem of each segment of the Pareto front. The Defining Initial Value Problem can be formulated in an explicit and in an implicit version. The implicit version is numerically more stable than the explicit version. We solve the Defining Initial Value Problem with standard explicit or implicit ODE methods. Changes in the active set, i.e., the determination of the segment ends of the Pareto frontier, are detected automatically via an appropriate switching function. The software has been implemented in `Matlab`®. For two academic benchmark problems we have shown numerically that the proposed method delivers—with comparable numerical effort—solutions with comparable or higher accuracy than existing methods like the NBI method. The accuracies for the results of the more difficult example are better by one to three orders of magnitude.

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